SACADA Database Code: 523

Topology: 4^2T285

# of independent nodes (IN): 2
Transitivity: [2553]
Space Group: Pbcn
Pearson: oP16
Coordination Number (CN): 4

Year: 2019

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
4^2T285 (SACADA #523)		3.475		0.470	408.3	450.5	84.1	SACADA[1]
4,4T285		3.449	2.61		428	465	77	doi: 10.1038/s41598-019-42483-5

Elasticity tensor (kBar)[1]

9284.6830	855.6347	1152.7210	-0.0000	0.0000	0.0000
855.6347	9790.8801	1215.1709	-0.0000	-0.0000	0.0000
1152.7210	1215.1709	11404.0850	-0.0000	-0.0000	0.0000
0.0000	0.0000	-0.0000	3302.5396	-0.0000	0.0000
0.0000	0.0000	-0.0000	-0.0000	5121.6141	-0.0000
-0.0000	0.0000	-0.0000	0.0000	-0.0000	5371.7534

[1] We apply the density functional theory (DFT) approach by using the Vienna Ab Initio Simulation Package (VASP) to calculate the total energy and properties of carbon allotropes.

DFT calculations

We apply the density functional theory (DFT) approach by using the Vienna Ab Initio Simulation Package (VASP) package [6] to calculate the total energy of carbon allotropes. The Generalized Gradient Approximation [7] (GGA) for exchange-correlational functional is used everywhere. The energy cutoff set to 600 eV. Fully automatic Γ-centered k-points mesh with a reciprocal-space resolution of $2\pi \times 0.025$ Å^{-1} is applied. We used tetrahedron method with Blöchl corrections to perform the k-point integration. The convergence thresholds are set at 10^{-6} eV for energy and 10^{-5} eV Å^{-1} for ionic forces. Polycrystalline elastic moduli — the bulk modulus, the shear modulus, Young's modulus, and the Poisson's ratio ν — have been calculated within the Voigt–Reuss–Hill [8] approximation. The Vicker's hardness H_v has been estimated according to Oganov's model [9].